Journal of Computational and Applied Mathematics 19 (1987) 151–160
North-Holland

On certain applications of two-point Padé type approximants with a single pole

Pablo GONZÁLEZ-VERA
Departamento Ecuaciones Funcionales, Universidad de La Laguna, Canary Islands, Spain

Received 7 February 1986

Abstract: In this paper several examples belonging to different topics in Numerical Analysis are considered, making use of certain two-point Padé type Approximants with a single pole. Results about convergence and error estimations are given.

1. Theory

Two-point Padé type approximants (in order to simplify the notation we shall write 2PTA's) were introduced by Draux [1] and Van Iseghem [2]. Recently, a formal study in the context of a noncommutative algebra has been made by Draux [3]. At the same time González-Vera [4] has carried out a treatment of these approximants in connection with Stieltjes series.

Let us give the precise definition of a 2PTA according to Draux. Given two formal power series

$$f_0 = \sum_{j=0}^{\infty} c_j z^j \quad (z \to 0) \quad \text{and} \quad f_\infty = \sum_{j=1}^{\infty} c_{-j}^* z^{-j}, \quad z \to \infty$$

and two nonnegative integers m and k $(0 \leqslant k \leqslant m)$, if $\tilde{P}_{km}$ is an arbitrary polynomial of degree m, then the rational function

$$f_{km}(z) = \tilde{Q}_{km}(z)/\tilde{P}_{km}(z) = \sum_{j=0}^{m-1} a_j z^j \bigg/ \sum_{j=0}^{m} b_j z^j$$

where the coefficients $\{a_j\}$ are determined by imposing

$$f_0 - f_{km} = \mathrm{O}(z^k) \quad \text{and} \quad f_\infty - f_{km} = \mathrm{O}\big((z^{-1})^{l+1}\big)$$

$(l = m - k)$, is said to be a (k/m) two-point Padé type approximant to the pair (f_0, f_∞), and we shall write

$$f_{km}(z) = (k/m)_{(f_0, f_\infty)}(z).$$

Let $f(z)$ be a function analytic on neighbourhoods of $z = 0$ and $z = \infty$, f_0 and f_∞ being the respective series expansions and introduce the linear functional D, defined on the space of the Laurent polynomials

$$D(x^j) = d_j = \begin{cases} c_j & \text{if } j \geqslant 0, \\ -c_j^* & \text{if } j < 0, \end{cases} \quad \text{for all } j \in Z.$$

Leting $V(t) = t^{-l} P_{km}(t)$, where $P_{km}(t) = t^m \tilde{P}_{km}(t^{-1})$, then the following error expression can be established [5].

Theorem 1.

$$f(t) - (k/m)_{(f_0, f_\infty)}(t) = \frac{t^k}{\tilde{P}_{km}(t)} D\left(\frac{V(x)}{1 - xt}\right).$$

We next give an expression of the error in terms of a complex integral. Let f be an holomorphic function in the simply connected regions D' and D'', containing respectively the origen and ∞.

By using Cauchy Integral Formula, we have

$$f(t) = \frac{1}{2\pi i} \int_{C'} \frac{f(t')}{t' - t} dt' \quad (t \text{ interior to } C');$$

on the other hand,

$$f(t) = \frac{1}{2\pi i} \int_{C''} \frac{f(t')}{t' - t} dt' \quad (t \text{ interior to } C'');$$

here C' and C'' are conveniently oriented.

With the transformation $t' = 1/x$, we have

$$f(t) = \frac{1}{2\pi i} \int_{C_0} \frac{x^{-1} f(x^{-1})}{1 - xt} dx = D\big((1 - xt)^{-1}\big), \quad t \to 0$$

and

$$f(t) = \frac{1}{2\pi i} \int_{C_\infty} \frac{x^{-1} f(x^{-1})}{1 - xt} dx = D\big((1 - xt)^{-1}\big), \quad t \to \infty,$$

where the functional D acts on the variable x, t being a parameter and C_0 and C_∞ represent the respective images of C' and C'' through the transformation $t' = 1/x$. Therefore, the following representation of the functional D has been deduced

$$D(F(x)) = \frac{1}{2\pi i} \int_C x^{-1} f(x^{-1}) F(x) \, dx.$$

Thus, by Theorem 1, one has:

Theorem 2.

$$f(t) - f_{km}(t) = \frac{t^k}{\tilde{P}_{km}(t)} \frac{1}{2\pi i} \int_C \frac{V(x) x^{-1} f(x^{-1})}{1 - xt} dx, \tag{1.1}$$

where C represents a closed path contained in a neighbourhood of the infinity when t is small, and a neighbourhood of the origen when t is large. [1]

Remark. Expression (1.1) is a consequence of the slightly more general following result. Let D be a closed region or several closed regions, that is, $D=\bigcup_1^p D_j$, and let its boundary Γ consists of a finite number of nonintersecting rectificable Jordan curve Γ_j. Let the points $t=0$ and $t=\infty$ be interior to D, and let the function $f(t)$ be analytic in D. If $f_{km}(t)$ denotes a two-point Padé type approximant with poles $\alpha_1, \alpha_2, \ldots, \alpha_m$ ($\alpha_i \neq 0$; $\alpha_i \neq \infty$), then we have

$$f(t)-f_{km}(t)=\frac{1}{2\pi \mathrm{i}} \int_{\Gamma_j} \frac{t^k \tilde{P}_{km}(x)}{x^k \tilde{P}_{km}(t)} \frac{f(x)}{x-t} \mathrm{d}x \tag{1.2}$$

t interior to D_j; $t \neq \alpha_j$ and $\tilde{P}_{km}(t)=\prod_1^m(t-\alpha_j)$

To check this, it is enough to use the error formula given by Walsh [6] for the problem of the rational interpolation by functions of the form

$$r(t)=\sum_{j=0}^{n} a_j t^j \Big/ \prod_1^m (t-\alpha_j)$$

of an analytic function $f(t)$ in n interpolatory knots. This result also holds for infinite regions [6, pp. 186–187]).

2. A preliminary example

The function $f(t)=(1-\mathrm{e}^{-t})/t$ is analytic in $\mathbb{C}$, and its McLaurin series is given by

$$f(t)=\sum_{n=0}^{\infty} \frac{(-1)^n t^n}{(n+1)!}=f_0. \tag{2.1}$$

In [2], 1PTA's to f_0 are considered, using as denominator $(1+x/n)^n$. On the other hand, McCabe [7] also studied this function via two-point Padé approximants (he used continued fractions) since for x tending to infinity in the right half-plane, one has

$$f(t) \sim 1/t=f_\infty. \tag{2.2}$$

We now give a result for 2PTA's to the pair (f_0, f_∞) with denominator $(1+x/m)^m$.

Theorem 3. *The sequence* $(m-1/m)_{(f_0, f_\infty)}(t)=\tilde{Q}_m(t)/(1+t/m)^m$, *converges uniformly to* (2.1) *on any compact of the complex plane.*

Proof. Let r be a positive real number and $t \in \mathbb{C}$, such that $|t|<r$. Then, by using (1.1), one has

$$|E_m(t)|=|f(t)-(m-1/m)_{(f_0, f_\infty)}(t)| \leqslant \frac{(1+r/m)^m(\mathrm{e}^r+1)|t|^{m-1}}{|1+t/m|^m(1-|t|/r)r^m}.$$

[1] This is because the contours C_0 and C_∞ used in this representation are the inverse of the contours C' and C'' of the Cauchy's formula used before (or the Γ's of the alternative proof of the remark coming after Theorem 2).

Table 1

x	$\lvert 1/1\rvert_{(f_0,f_\infty)}$	$(2/3)_{(f_0,f_\infty)}$	$\lvert 0/1\rvert_{f_0}$	Exact
0.5	0.666666	0.72000	0.80000	0.79694
1	0.500000	0.55555	0.66666	0.63212
2	0.333333	0.37500	0.50000	0.43233
4	0.200000	0.22222	0.33333	0.24544
6	0.142850	0.15625	0.25000	0.16649
8	0.11111	0.12000	0.20000	0.12589
10	0.9090	0.09722	0.16666	0.09999

Table 2

x	$\lvert 1/1\rvert_{(f_0,f_\infty)}$	$(2/3)_{(f_0,f_\infty)}$	$\lvert 0/1\rvert_{f_0}$	Exact
0.1	0.90909	0.92970	0.95238	0.95162
0.2	0.83333	0.86776	0.90909	0.90634
0.3	0.76923	0.81285	0.86956	0.86393
0.4	0.71428	0.76388	0.83333	0.82419

Table 3

x	$\lvert 0/2\rvert_{f_0}$	$\lvert 1/2\rvert_{(f_0,f_\infty)}$	$(3/4)_{(f_0,f_\infty 0}$
0.5	$0.6\cdot 10^{-4}$	$0.93\cdot 10^{-3}$	$0.23\cdot 10^{-3}$
2	$0.376\cdot 10^{-2}$	$0.121\cdot 10^{-1}$	$0.182\cdot 10^{-2}$
4	$0.146\cdot 10^{-1}$	$0.155\cdot 10^{-1}$	$0.562\cdot 10^{-2}$
6	$0.234\cdot 10^{-1}$	$0.152\cdot 10^{-1}$	$0.385\cdot 10^{-2}$
8	$0.302\cdot 10^{-1}$	$0.959\cdot 10^{-2}$	$0.562\cdot 10^{-2}$
0	$0.302\cdot 10^{-1}$	$0.959\cdot 10^{-2}$	$0.621\cdot 10^{-2}$

ecause, in this case $V(x)=x^k(1+1/mx)$; $(k=m-1)$. Let K be an arbitrary compact, $=\overline{D}(0, r_0)=\{\,\lvert t\rvert \leqslant r_0\}$, and make $r=2r_0$, then

$$\lvert E_m(t)\rvert \leqslant 2\,\mathrm{e}^{3r_0}(\mathrm{e}^{2r_0}+1)\left(\tfrac{1}{2}\right)^{m-1}.$$

ence, the uniform convergence is warranted. [2]

Some numerical results are shown in Tables 1–3.

As one can see, the best global approximation corresponds to 2PTA's column. If t is close to ro, the Padé approximant in one point is superior, according to Table 2.

However the 2PTA is better than the 2PA (Classical two-point Padé approximant)

By using three coefficients in (2.1), we get the comparative Table 3 on absolute errors, in the terval [0, 10].

ctually, for large t, the bound is useless, because, the example is not analytical in a neighbourhood of ∞ (as most f the interesting examples) so that, Theorem 2 cannot be used with C. However, the numerical demonstrations upply a more optimistic information.

3. Thomas Fermi's equation

Let the function $y=f(x)$, $x \in [0, \infty)$ be, the solution of Thomas Fermi equation

$$y''=y^{3/2}x^{-1/2}, \qquad y(0)=1, \quad \lim_{x\to\infty} y(x)=0. \tag{3.1}$$

This function provides a description of the charge density in atoms with a high atomic number. Kobayashi et al. [7] computed the value -1.5880710 for $f'(0)$, hence (3.1) can be seen as an initial value problem. On the other hand, Mason [9] obtains for $f(x)$ a power series in the variable $t=x^{1/2}$ in the form

$$f \sim f_0 = c_0 + c_1 t + c_2 t^2 + \cdots, \quad t \to 0 \tag{3.2}$$

where $c_0=1$, $c_1=0$, $c_2=f'(0)$, etc.

With respect to the behaviour of $f(x)$ for x tending to infinity, it can be seen that [10]

$$f \sim 144/x^3, \quad x \to \infty. \tag{3.3}$$

Now we are going to use 2PTA's in order to get a global approximation to $f(x)$ from (3.2) and (3.3). Here we should note that Mason used Padé approximants in one point, probably because he did know an appropriate definition of 2PA for the series (3.2) and (3.3). However, the recent paper by Draux [3]—enables us to define 2PTA for (3.2) and (3.3).

Since $f(x)>0$ in the interval $[0, \infty)$, it will be useful considering approximants in the form $F_m(t)=f_m^2(t)$, where f_m represents an approximant to the function $g^{1/2}$ and $g(t)=f(t^2)$. Thus,

$$\begin{aligned} g(t) &\sim c_0 + c_1 t + c_2 t^2 + \cdots, && t \to 0,\\ g(t) &\sim 144/t^6, && t \to \infty. \end{aligned}$$

Letting $h(t)=(g(t))^{1/2}$, one has

$$\begin{aligned} h(t) &\sim d_0 + d_1 t + d_2 t^2 + \cdots, && t \to 0,\\ h(t) &\sim 12/t^3, && t \to \infty, \end{aligned} \tag{3.4}$$

The coefficients $\{d_j\}$ are given recursively by

$$d_0 = c_0^{1/2}, \qquad d_k = (kc_0)^{-1} \sum_{i=0}^{k-1} \left(\frac{k-i}{2} - i \right) d_i c_{k-i}, \quad k \geqslant 1,$$

and the coefficients $\{c_j\}$ $(j \geqslant 3)$ can be calculated according to the scheme

$$c_{n+1} = 4e_{n-2}/(n^2-1), \quad n \geqslant 2,$$

where $e_0=(c_0)^{3/2}$, and

$$e_k = (kc_0)^{-1} \sum_{i=0}^{k-1} \left(\tfrac{3}{2}(k-i) - i \right) e_i c_{k-i}, \quad k \geqslant 1.$$

Now, making use of approximants with denominator $(1+x/\alpha(m))^m$ $(\alpha(m)>0)$, if we impose the maximum absolute error be less than 5.10^{-5} in the interval $[0, 1000]$, it is enough to take $m=12$, and $\alpha(12)=0.45525$ (we use (1.1) to compute the error bound). So, we have got the same accuracy that one Mason's [11], via Padé approximants in one point in the form $|r/(r+3)|$

Table 4

x	Approximation	Exact value
0.1	0.881696	0.8817
0.4	0.659532	0.6596
0.8	0.484887	0.4849
2	0.242847	0.2430
5	$0.788321\cdot10^{-1}$	$07881\cdot10^{-1}$
8	$0.365924\cdot10^{-1}$	$0.3659\cdot10^{-1}$
20	$0.578536\cdot10^{-2}$	$0.5785\cdot10^{-2}$
50	$0.643046\cdot10^{-3}$	$0.6323\cdot10^{-3}$
100	$0.109325\cdot10^{-3}$	$0.1002\cdot10^{-3}$
500	$0.127431\cdot10^{-5}$	$0.1034\cdot10^{-5}$
1000	$0.168651\cdot10^{-6}$	$0.1351\cdot10^{-6}$

with $r=4$, that is, he required 12 coefficients in (3.4). In our case, $m=12$, and we only need 9 coefficients in (3.4).

Table 4 presents the numerical results.

4. Dawson's integral

We are concerned with Dawson's integral

$$F(x)=\mathrm{e}^{-x^2}\int_0^x \mathrm{e}^{t^2}\,\mathrm{d}t, \tag{4.1}$$

which is very important in several physical problems. It occurs in such applications as heat conduction, spectroscopy and in the theory of electrical oscillations in certain special vacuum tubes. The function $F(x)$ was first tabulated by Dawson [12]. Since then, extensive tabulations have been given by different authors (see [13] for more details).

Differentiating (4.1) we readily obtain the MacLaurin series

$$F(x)=\sum_{k=0}^{\infty} c_k 2^k x^{2k+1},\quad c_k=\frac{(-1)^k}{1\cdot3\cdot5\cdots(2k+1)}. \tag{4.2}$$

When $|\arg(x)|<\frac{1}{4}\pi$, approximations to $F(x)$ for large value of $|x|$ can be obtained from the asymptotic expression

$$F(x)\sim\sum_{k=1}^{\infty}\frac{d_k}{2^k x^{2k-1}}$$

$$d_k=1\cdot3\cdots(2k-3),\quad k\geqslant2,\qquad d_1=1. \tag{4.3}$$

This series is divergent for all real values of x, but provided it is truncated after a suitable number of terms, supply good approximations to Dawson's integral.

From (4.2) and (4.3) 2PTA's will be considered in order to estimate (4.1). For this purpose let us introduce the formal series

$$L(x)=\sum_{k=0}^{\infty}\frac{(-1)^k x^k}{1\cdot3\cdot5\cdots(2k+1)}\quad\text{and}\quad L^*(x)=\frac{1}{x}+\sum_{k=2}^{\infty}\frac{1\cdot3\cdots(2k-3)}{x^k}.$$

Let us consider the sequence

$$f_{km}(x) = (k(m)/m)_{(L,L^*)}(x) = Q_{k(m)}(x)/(1+x/m)^m,$$

such that $0 \leqslant k(m) \leqslant m$; $\lim_{m\to\infty} k(m) = \infty$ and $\mathrm{Inf}\{k(m)/m\} > 0$.

Making $F_{k(m)}(x) = x f_{k(m)}(2x^2)$, the next result holds.

Theorem 4. *The sequence* $\{F_{k(m)}(x)\}$ *converges uniformly to* $F(x)$ *on any interval* $[0, b]$.

Proof. First, it can be easily proved that $F_{k(m)}$ constitutes a $(2k(m)/2m)$ 2PTA to (4.2) and (4.3).

Let us write $E_m(x) = f(x) - f_{k(m)}(x)$ and $E'_m(x) = F(x) - F_{k(m)}(x)$ where f is a function admitting the expansions L and L^* for x close to zero and x sufficiently large respectively.

Let K' be a compact of $\mathbb{C}$, $K' \subset \overline{D}(0, r_0)$, then

$$\forall x \in K' \quad |E'_m(x)| \leqslant r_0 |E_m(2x^2)| = r_0 |E_m(t)|, \quad \text{where } t = 2x^2 = \Phi(x).$$

As $|F(x)| \leqslant |x| \exp|x|^2$, so that $|f(t)| \leqslant \exp\frac{1}{2}|t|$, and $V(x) = x^{k(m)}(l + 1/mx)^{k(m)}$ (as in Theorem 3), then from (1.1), with $|x| = 1/R$, one has

$$|E_m(t)| \leqslant |t|^{k(m)}(1 - |t|/m)^{-m} R^{-k(m)}(1 + R/m)^m \exp(R/2)(1 - |t|/R)^{-1}.$$

Therefore,

$$|E_m(t)| \leqslant \exp\left(R_0 + \tfrac{3}{2}R\right)(R_0/R)^{k(m)}/(1 - R_0/R) \quad \text{when } |t| \leqslant R_0 < R$$

and $R_0 \ll m$.

From (1.1), we get

$$\sup_{t\in K} |E_m(t)| \leqslant \frac{\exp\left(\frac{3}{2}R_0\right)}{1 - R_0/R}(R_0/R)^{k(m)}, \quad R > R_0. \tag{4.4}$$

Thus, by (4.4) we can get uniform convergence on any bounded interval in $[0, \infty)$. Furthermore, we have

Theorem 5. *The sequence* $\{F_{k(m)}\}$ *converges faster than geometrically to* $F(x)$ *in* $[0, b]$ $(\forall b > 0)$.

Proof. From Theorem 4, making $\lambda = R/R_0$, one has

$$\sup_{t\in K} |E_m(t)| \leqslant \operatorname*{Inf}_{\lambda>1} |H_m(\lambda) \quad \text{where } H_m(\lambda) = \frac{e^{3R_0/2}}{(\lambda-1)\lambda^{k(m)-1}}.$$

It is not difficult to see that $H'_m(\lambda)$ vanishes at two real points λ_1 and λ_2 (it can be assumed $\lambda_1 < 1 < \lambda_2$)

Since $\lim_{\lambda\to 1^+} H_m(\lambda) = \infty$, $H'_m(\lambda) > 0$ $(\forall \lambda > \lambda_2)$ and $\lim_{\lambda\to\infty} H_m(\lambda) = \infty$, then the minimum must be located at $\lambda = \lambda_2$, satisfying

$$\lambda_2 < \lambda' = 1 + 2k(m)/3R_0.$$

Hence, $\mathrm{Inf}_{\lambda>1} H_m(\lambda) < H_m(\lambda')$, and it can be established finally

$$\lim_{m\to\infty} |H_m(\lambda')|^{1/m} = 0.$$

Consequently, one gets $\lim_{m\to\infty}[\sup_{t\in K}|E_m(t)|]^{1/m}=0$. So, if $0<b<+\infty$,

$$\lim_{m\to\infty}\left[\sup_{t\in[0,\,b]}|F(x)-F_{k(m)}(x)|\right]^{1/m}=0.$$

Therefore, the geometric convergence has been warranted.

5. An application to Laplace transform inversion

As it is well known, many techniques in the Numerical Inversion of Laplace Transform consist of determining rational approximations (Padé Approximants, for example) to

$$\bar{f}(p)=\int_0^\infty \mathrm{e}^{-pt}f(t)\,\mathrm{d}t$$

provided that expansions for $\bar{f}(p)$ at $p=0$ or $p=\infty$ are known, and next these rational functions are inverted analytically.

The procedure gives satisfactory results when the expansions of the function $\bar{f}$ are in integer powers in the variable p, which happens in a restricted number of cases.

A possible alternative is to deduce an expansion for $\bar{f}(p)$ in the form

$$\bar{f}(p)\sim\sum_{n=1}^{\infty}c_n p^{-\lambda_n},\qquad p\to\infty,\quad 0<\lambda_1<\lambda_2\cdots$$

and then inverting term to term. In this fashion, a power series for $f(t)$ as $t\to 0$ can be obtained. If Padé approximants are used now, then one has certain approximants to the inverse transform $f(t)$. However, in this case, the convergence is usually, slow for t sufficiently large.

In this sense, 2PTA's constitute an extremely useful tool, when a global estimation of the inverse transform is required and an elementary expression for $\bar{f}(p)$ is not known.

Now, we are going to illustrate these observations with one of the examples given by Grundy [14], namely

$$\bar{f}(p)=1/\sqrt{p}\left(\sqrt{p}+a\right),\quad a>0.$$

In this case, one has

$$\bar{f}(p)=\frac{1}{p}\sum_{n=1}^{\infty}(-1)^n\left(ap^{-1/2}\right)^n,\quad |p^{1/2}|>a.$$

Hence, (see [15, p. 195 and p. 254]),

$$f(t)=\sum_{n=0}^{\infty}\frac{(-1)^n a^n t^{n/2}}{\Gamma\left(1+\frac{1}{2}n\right)}.$$

On the other hand,

$$\bar{f}(p)=\frac{1}{ap^{1/2}}\sum_{n=0}^{\infty}(-1)^n\left(\frac{p^{1/2}}{a}\right)^n,\quad |p^{1/2}|<a,$$

therefore,

$$f(t)\sim\sum_{n=0}^{\infty}\frac{(-1)^n t^{-(n+1)/2}}{a^{n+1}\Gamma\left(\frac{1}{2}(1-n)\right)}.$$

Letting $z=\sqrt{t}$ and $f(z^2)=g(z)$, then

$$g(z)=\sum_{n=0}^{\infty} c_n z^n = g_0,$$

with g analytic in C and where $c_n=(-1)^n a^n/\Gamma(1+\frac{1}{2}n)$. At the same time,

$$g(z)\sim \sum_{n=1}^{\infty} d_n z^{-n}=g_\infty, \qquad z\to\infty, \quad d_n=\frac{(-1)^n}{a^{n+1}\Gamma(\frac{1}{2}(1-n))}.$$

Grundy constructed certain continued fractions with respect to the pair (g_0, g_∞) and he obtained an error of about 10^{-8} making use of nine coefficients in both expansions. In this case the error is exactly known because the inverse transform is

$$f(t)=\mathrm{e}^{a^2 t}\operatorname{erfc}(a\sqrt{t}).$$

On the other hand, the approximations given by Grundy require quite complex algorithms for their computations.

We now use sequences of 2PTA's for the same problem. Their computation is simple and uniform convergence is attained.

Let

$$g_m(z)=(k(m)/m)_{(g_0,\,g_\infty)}(z)=\tilde{Q}_m(z)/(1+z/\alpha_m)^m,$$

$\alpha_m>0$, $\forall m$ and $\lim_{m\to\infty} m/\alpha_m=p$ (p as small as we want).

In these conditions, one has

Theorem 6. *The sequence* $\{g_m\}$ *converges to* $g(z)$ *uniformly on any compact of* $[0, \infty)$.

Proof. From (1.1), letting $C=\{x/|x|<1/r;\ r>0\}$, one gets

$$|E_m(z)|=|g(z)-g_m(z)|\leqslant \frac{(1+r/\alpha_m)}{|z/\alpha_m+1|^m}\,\frac{M(r)}{1-|z|/r} \tag{5.1}$$

where $M(r)=\sup_{t\in C'}|g(t)|$, and C' is the image of C by the transformation $z\to z^{-1}$.

Let r_0 be fixed, such that $|z|<r_0$ and $\mathrm{Re}(z)\geqslant 0$, then

$$|g(z)-g_m(z)|\leqslant \frac{\mathrm{e}^{pr}M(r)}{1-r_0/r}(r_0/r)^{k(m)} \quad \text{for any } r>r_0.$$

From (5.1) the uniform convergence in the interval $[0, r_0]$, $r_0>0$, is established.

Acknowledgments

I am deeply indebted to Professors Nàcere Hayek, Claude Brezinski and Luis Casasús for their kind guidance, valuable suggestions and helpful discussions during the preparation of this paper.

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